C:\Program Files\STNEXP\Queries\10570628.str chain nodes : 15 22 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 16 17 18 19 20 21 chain bonds : 1-15 15-16 15-22 ring bonds :

1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 5-12 6-7 6-14 8-9 9-10 10-11 12-13 13-14 16-17 16-21 17-18 18-19 19-20 20-21 exact/norm bonds : 1-2 1-7 1-15 3-4 4-5 5-6 5-12 6-7 6-14 12-13 13-14 15-22 exact bonds :

normalized bonds : 2-3 2-8 3-11 8-9 9-10 10-11 16-17 16-21 17-18 18-19 19-20 20-21

15-16

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS